



# Xcalibur Gemini

EXPERT TO SPECIALIST  
SMALL MOLECULE SYSTEMS

The Measure of Confidence



**Agilent Technologies**

# The Expert System

## Xcalibur E

### Perfect for the Expert crystallographer

The expert diffractometer for the modern chemical crystallography laboratory, the Xcalibur E is the most popular choice of system for single wavelength small molecule crystallography.

Most often configured with molybdenum radiation but also available with copper, the Xcalibur E system comprises a 4-circle kappa goniometer mounted with a single wavelength Enhance X-ray source and the Eos CCD detector. Incorporating the fastest, most sensitive CCD detector available today, the Xcalibur E is the perfect choice of diffractometer for both day to day routine crystal structure determinations and the more challenging high resolution electron density studies.



Xcalibur E goniometer with Enhance X-ray source and Eos CCD

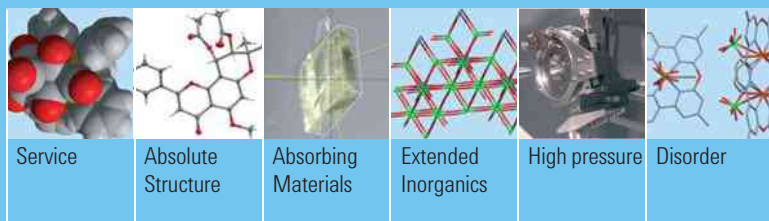
### Upgradeable

Since the future needs of your research may change, the Xcalibur E has been designed to be upgraded to a dual wavelength Gemini system through the addition of either a second Enhance or a high intensity Enhance Ultra X-ray source.



Gemini E goniometer with dual Enhance (Mo and Cu) X-ray sources

### Applications



Service

Absolute  
Structure

Absorbing  
Materials

Extended  
Inorganics

High pressure

Disorder

# The Specialist System

## Gemini A Ultra

### Ideal for Specialist crystallographic research

Ideal for both the specialist crystallographic researcher and for the centralised service laboratory, the Gemini is the world's most popular dual wavelength system.

The latest generation of Gemini, the Gemini A Ultra combines Agilent's fast, high performance and large active area ( $\varnothing 135$  mm) Atlas CCD detector with both a molybdenum Enhance and a high intensity copper Enhance Ultra X-ray source, co-mounted on a single 4-circle kappa goniometer.

While the molybdenum Enhance is ideal for routine small molecule experiments, the Enhance Ultra provides a high intensity copper X-ray beam, ideally suited to the study of the smallest, weakly diffracting samples.

Combining speed, dual wavelength, high sensitivity and large active area, the Gemini A Ultra is an extremely versatile system capable of a wide range of standard and specialist applications in small molecule and protein crystallography.



Gemini A Ultra with Enhance (Mo)(left front), Enhance Ultra (Cu) (left back) and Atlas CCD (right)

### Applications

Diffuse scatter	Twinning	Macro-molecules	Small weak crystals	Incommensurate	Quasi-crystals	Charge / electron density	Powders	Proteins

# Xcalibur & Gemini

## The System

The Xcalibur E and the Gemini A Ultra are supplied as turn-key single crystal diffraction systems. Each system occupies a footprint of approximately 1m<sup>2</sup> (excl. chiller unit) and is housed in a fully interlocked radiation proof and lead doped glass cabinet. Within the base of the system are housed the system interface, software controlled X-ray generators and compact CCD chiller unit.

The Gemini A Ultra incorporates two independent high voltage and air cooled X-ray generators. In the Xcalibur E only one such generator is present. However, the Xcalibur E is fully prepared for future upgrade to a dual wavelength system .

Separate from the main diffractometer unit, the Gemini A Ultra and the Xcalibur E are supplied with a stand alone system control computer, an LCD monitor and an X-ray tube water chiller unit.

The system control computer comes pre-loaded with Agilent's extremely powerful data collection, data reduction and processing software CrysAlis<sup>Pro</sup>, which can be extended to include automatic structure solution and refinement via the optional AutoChem software.



Complete Gemini A Ultra system  
with external X-ray chiller

# Single and Dual Wavelength X-ray Sources

## Kappa Goniometer

At the heart of the Xcalibur E and the Gemini A Ultra system is Agilent's 4-circle kappa goniometer which provides extremely high angular resolution Mo and Cu data, meeting and significantly exceeding the publication requirements of the IUCr journals.

For ease of sample mounting and alignment, the goniometer incorporates a rotatable beam stop and a 120x magnification video microscope which is linked to a dedicated LCD monitor within the system enclosure.

Motorised and software controlled, the theta axis detector mount accommodates all Agilent CCDs and allows the sample to detector distance to be quickly and easily adjusted to suit the experiment.

## Optional Cryo-Devices

The Xcalibur E and the Gemini A Ultra systems accommodate all major sample cooling devices including Agilent's open flow liquid nitrogen device (90-490K) and liquid helium, Helijet (<10-90K).

## Single wavelength X-ray source



Enhance X-ray source

The Enhance single wavelength X-ray source can be either molybdenum or copper radiation and is factory pre-aligned to give maximum intensity. Easy to use, this patented design comprises:

- A long fine focus ceramic X-ray tube (2.2 – 3 kW)
- Integrated fast X-ray shutter
- Pre-aligned monochromator
- Mono-capillary collimators (0.3 – 1.0 mm available)

## Dual wavelength X-ray source



Co-mounted Enhance (Mo) (front) and Enhance Ultra (Cu) (back) X-ray sources

Co-mounted alongside a molybdenum Enhance, the patented Enhance Ultra combines a copper, ceramic tube with a state-of-the-art multi-layer optic to provide a high intensity X-ray beam.

- 2.2 kW Cu sealed tube
- Approximately, 300 micron beam size
- Comparable data to a 5kW rotating anode with optics
- Multi-layer X-ray optic

# CCD detectors



Agilent Technologies, formerly as Oxford Diffraction, has been manufacturing and selling CCD detectors since 1992. As experts in CCD design and manufacture, with patented mounting technology, all our detectors are purpose built specifically for X-ray diffraction as part of a complete diffractometer system.

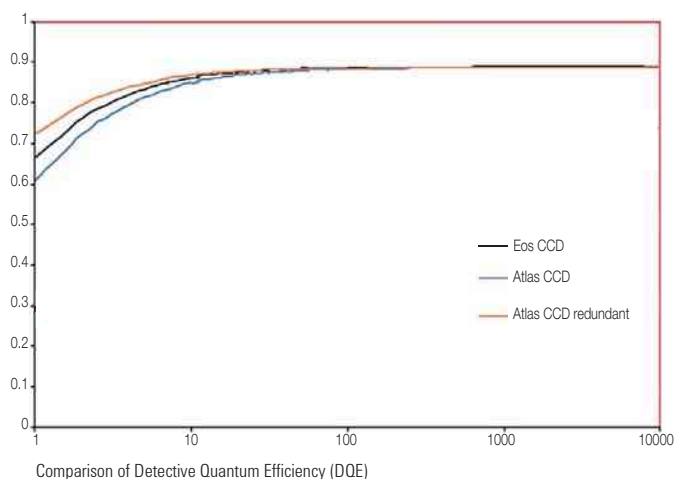
There are a number of key factors to consider when designing a modern CCD detector for today's experimental crystallographer. These factors should be considered as a whole rather than independently, since the detector is a collection of components and not just a CCD chip. The key factors are:

**Speed** – The 'frame to frame time' or 'duty cycle' is the actual time taken to read-out the CCD chip, digitise the data and write the data to the storage device. This cycle time is often significantly longer than the chip read-out time quoted by many manufacturers. For Agilent's Atlas and Eos detectors, the duty cycle is only 0.28 sec in 512 x 512 pixel mode, which is only 0.13 sec longer than the chip read-out time, making Agilent's CCDs the fastest CCD detectors currently available.

**Sensitivity** – The ability to measure signal (reflections) above background is the Detective Quantum Efficiency (DQE) of the detector. As indicated by the plot of DQE versus the number of X-ray photons in a reflection, Agilent CCD detectors have a high DQE ranging from 0.6 to 0.85 (where the limit is 1.0) depending on strength of signal, and thus deliver outstanding sensitivity when measuring both strong and weak signals.

**Gain** – The conversion rate of X-ray photons to electrons is referred to as gain. Generally speaking the larger the gain figure the better, as this indicates a greater conversion of X-ray photons to electrons by the CCD. The Agilent Eos and Atlas with Mo gains of 330 and 180 e-/X-ray respectively are the highest currently available.

**Precision** – This relates to the precision of conversion of every X-ray image to a digital signal. Every image and every signal within that image is broken down into blocks of data 'bits'. The greater the number of hard wired bits (not software) the greater the number of blocks the data is digitised into and as a result the higher the precision of the data collected. At 18 bits hard wired, the Atlas and Eos are the highest precision CCD detectors currently available from any manufacturer.



## Atlas



The Atlas CCD represents the optimum combination of large active area size (Ø135 mm) and detector sensitivity. The Atlas is the ideal choice of CCD for fast, high quality data collection using both Mo and importantly Cu radiation where small molecule data is typically sparsely spread within reciprocal space.

- Active area Ø135 mm
- Speed, 0.28 sec (duty cycle)
- Sensitivity, 40% higher
- Gain, 180 e-/X-ray (Mo)
- Precision, 18 bit (hard wired)
- Low noise

## Eos



The Eos CCD combines the highest gain CCD (330 e-/X-ray) of any manufacturer with the highest precision and fastest duty cycle speed. The most sensitive CCD detector available today, the Eos is the best choice for single wavelength, molybdenum applications.

- Active area 92 mm diagonal
- Speed, 0.28 sec (duty cycle)
- Sensitivity, 40% higher
- Gain, 330 e-/X-ray (Mo)
- Precision, 18 bit (hard wired)
- Low noise

**Dynamic Range** – This describes a system's ability to measure strong and weak signals simultaneously on the same range. This is defined as the full well capacity over the total noise. For the Atlas and Eos the dynamic range is  $\geq 50,000$  and is equal to or higher than any other CCD detector.

**Low Noise** – The noise of a CCD detector is a combination of the read noise of the CCD chip, the combined noise of the detector electronics and the dark current noise. The dark current is typically insignificantly low and for routine small molecule crystallography, where exposure times are considerably  $< 20$  min, the dark current is so low it can be ignored. The noise of the detector then relates purely to the read noise and electronic noise. All Agilent detectors are built around low noise CCD chips and are optimised for very low noise electronics.



The Xcalibur comes complete with CrysAlis<sup>Pro</sup>, Agilent's intelligent data collection and data processing software for small molecule and protein crystallography. Designed around an easy to use graphical user interface, CrysAlis<sup>Pro</sup> can be operated under fully automatic, semi-automatic or completely manual control.

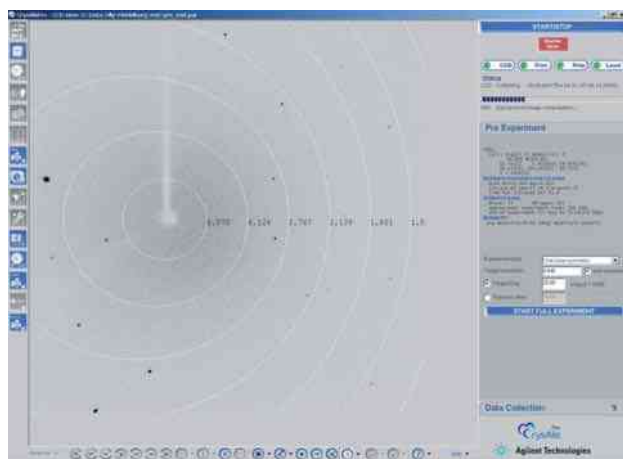
### Automatic crystal screening

At the heart of CrysAlis<sup>Pro</sup> are the automatic crystal screening, data collection and strategy software modules. For a typical crystal, a short pre-experiment lasting less than 5 minutes is recorded to evaluate the crystal quality. From the first frame of data, CrysAlis<sup>Pro</sup> automatically evaluates the crystal quality and provides the user with information regarding the unit cell, intensity estimation by resolution range and suggested frame exposure times for the full data collection.

### Fastest Strategy software

Following the pre-experiment, the sophisticated CrysAlis<sup>Pro</sup> strategy software automatically calculates the optimal conditions for fast, high quality, complete data collection. No pre-defined strategies are used. Instead, all strategies are calculated based on the specific crystal orientation and unit cell. The user has complete control to optimise the strategy for a wide variety of targets including multiplicity, time and resolution. In addition a series of restraints and constraints can be applied. The strategy calculations are extremely fast and efficient allowing the user to quickly adapt the data collection conditions with Mo or Cu radiation.

Experiments can also be designed to automatically collect data at multiple, user-defined temperatures (interfacing with any cryodevice). The same facility can also be used to run back-to-back Cu and Mo experiments on Gemini systems.



Main CrysAlis<sup>Pro</sup> GUI



# AutoChem Software



**AutoChem is the ultimate in fully automatic structure solution and refinement programmes for chemical crystallography.**

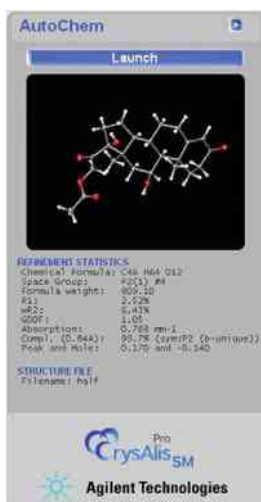
Developed exclusively for Agilent Technologies by the authors of OLEX2 (Durham University, UK), AutoChem adopts an entirely new approach to the automation of crystal structure determination and is seamlessly integrated into Agilent's CrysAlis<sup>Pro</sup> software providing real time structure solution and refinement during data collection.

Since its launch in 2006, CrysAlis<sup>Pro</sup> has provided automatic data collection and concurrent data reduction. Now using AutoChem, CrysAlis<sup>Pro</sup> completes the crystal structure determination.

AutoChem runs continuously throughout data collection providing the user with visual feedback within the main CrysAlis<sup>Pro</sup> GUI. This feedback is presented in the form of an interactive 2-D model of the crystal structure alongside key refinement results including R factor, Goodness-of-fit and absolute structure parameter.

Should the user wish to review the structure more closely or to control aspects of the structure solution, a full version of OLEX2 complete with AutoChem plugin can be launched at any time from within CrysAlis<sup>Pro</sup>. Using OLEX2, the user is able to review all aspects of the refinement, step back to any stage of the process and apply changes as necessary.

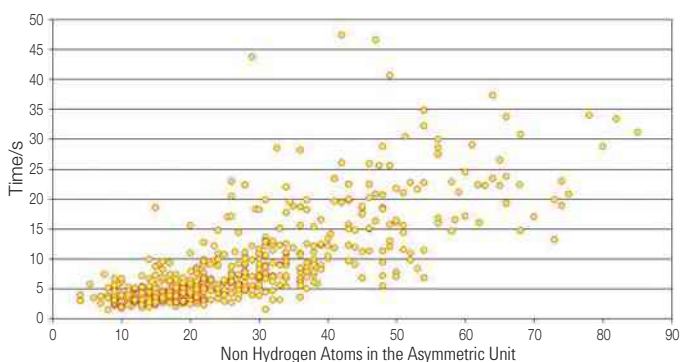
For standard crystal structures, AutoChem dramatically speeds up the process of structure solution, refinement and report generation. Developed using >2000 structures, AutoChem determined the majority of the tested routine structures in under 15 sec from solution to final report.



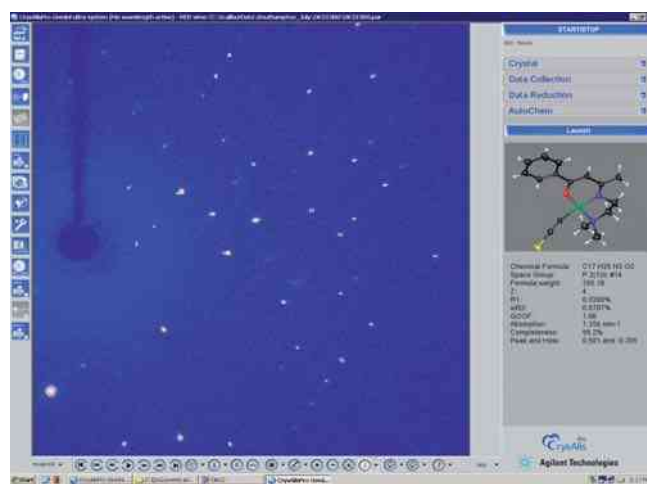
AutoChem Software

An intelligent programme, AutoChem selects the best method of structure solution, be it Patterson, direct methods or charge flipping. Using the speed and power of SMTBX<sup>1</sup> based refinement as standard but with options for SHELX, AutoChem refines the structure, accurately assigning atom types based on geometry. Atoms are modelled anisotropically where the data supports it and hydrogen atoms are included in calculated geometric positions. The structure is then re-labelled and refined to completion before a final html based structure report is generated.

- Fully automated structure solution, refinement and report generation
- Fully integrated with data collection software
- Developed using >2000 structures
- Majority of routine tested structures completed in under 15 sec
- Full user interaction and intervention possible at anytime
- AutoChem is exclusive to Agilent Technologies



Time for routine structure solution and refinement based on recent trials



CrysAlis<sup>Pro</sup> with integrated AutoChem feedback panel

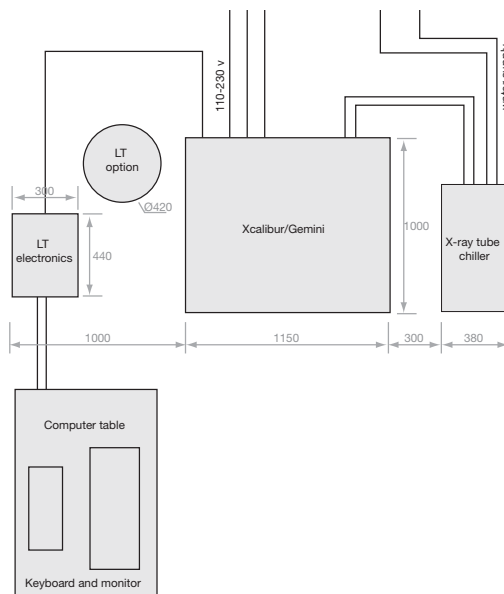
# Xcalibur Gemini

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SMALL MOLECULE SYSTEMS

## Technical Specifications



Suggested system layout (in mm)



## Environmental requirements

Power	230 / 110 V $\pm$ 10% 1x 16 A fuse protected 1x 32 A fuse protected (for each X-ray generator)
Water supply	2 l/min flow required 3 – 5 bar gauge 10 – 20 °C range Drain required
Relative Humidity	<80 % non-condensing
Weight loading	Able to bear system weight of ~500 kg over an area of 0.64 m <sup>2</sup>
Temperature	18 – 23 °C

Please refer to the system user manual for the most up to date and complete requirements.

For more information on Agilent Technologies' X-ray Products please contact us at: **XRDsales@agilent.com**

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Printed in U.S.A., December 7, 2010  
SI-2499

